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CHEMICAL & ENGINEERING
NEWS

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ACS national meeting in Atlanta
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Abortion debate clouds future of promising pharmaceutical
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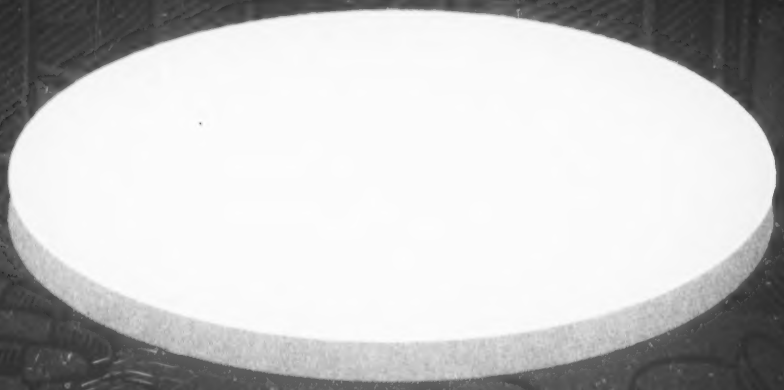

CHEMICAL & ENGINEERING
NEWS
MARCH 11, 1991

Volume 69, Number 10
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Final Program

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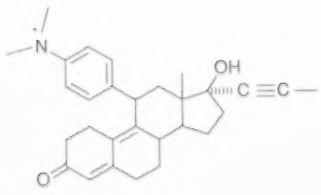

RU-486

News Focus

RU-486, a progesterone antagonist developed in France and used to terminate pregnancy, is potential anticancer and anti-Cushing's agent, but abortion controversy hinders U.S. research on it. **Page 7**

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LETTERS

CHEMICAL SAFETY

Explosions from organic azides, peroxides

I wish to report two incidents that may be of interest. In the first, a 25-g preparation of 1,4-diazido-2-butene exploded during purification by high-vacuum short-path distillation. The distillation temperature had reached approximately 70 °C in the pot when the explosion occurred. At the time of the explosion, one employee had removed the shielding to prepare to shut down the operation. This employee received facial burns and lacerations, but safety glasses prevented permanent eye injury. A second employee across the room received a minor laceration from flying glass. The force of the explosion destroyed the distillation apparatus and nearby glassware, spilling methanol, oil, and about 50 mL of mercury.

Organic azides are known to exhibit dangerous instability, especially those containing unsaturated carbon-carbon bonds and more than one azido group. Heat, shock, and traces of strong acids or metallic salts may trigger explosive decomposition. These compounds must be handled with extreme caution on a small scale, while ensuring the protection of employees and surrounding equipment in the event of an explosion. It should be noted that this material had been distilled in this fashion without incident several times previously, illustrating the unpredictable nature of these substances.

The second incident involved a 500-mL bottle of peracetic acid packaged with what appeared to be paper absorbent in a metal shipping container. The container had been placed on its side, allowing liquid to leak through the bottle's vented cap (peracetic acid bottles are vented to allow release of the pressure that builds up from the normal slow decomposition of the material). The spilled liquid reacted exothermically with the absorbent, heating the metal can until it became quite hot to the touch. Luckily, the heat generated did not trigger any further reaction. Heating peracetic acid above 65 °C may cause self-accelerating decomposition, and temperatures above 110 °C will cause violent explosion. This incident emphasizes the importance of ensuring compatibility between packaging materials and reactive chemicals such as peroxides.

Bruce I. Tobias
Chemical Safety Officer
Environmental Control & Research Program, Frederick Cancer Research & Development Center
Frederick, Md.

Editor's note: Numerous references to the instability of organic azides will be found in the literature, including the fourth edition of "Bretherick's Handbook of Reactive Chemical Hazards" [Butterworth-Heinemann, Stoneham, Mass. (1990)].

Stereochemical puzzle

I would like to draw attention toward the excellent comment by Ernest Eliel and Samuel Wilen on the term homochirality (C&EN, Sept. 10, 1990, page 2). I quite agree with my distinguished colleagues, since homochiral doesn't mean strictly enantiomerically pure.

This is another example of the increasing stereochemical puzzle, where there is an almost babel-like confusion. Terms like stereoselective, stereospecific, chemo- or regioselective, among others, are often defined in different ways—and, unfortunately, are not completely unambiguous. Another interesting dichotomy emerges from the dynamic stereochemistry. The widely used term of asymmetric synthesis was first introduced by Marckwald [*Ber.*, 37, 1368 (1904)], as the process of forming an optically active compound through the reaction of an achiral substrate with a (homo)chiral reagent. A broader definition can be found in "Asymmetric Organic Reactions" by James D. Morrison and Harry S. Mosher [Prentice-Hall, Englewood Cliffs, N.J. (1971)]. Curiously, the term asymmetric induction was coined later [McKenzie and Ritchie, *Biochem. Z.*, 237, 1 (1931)] to describe the chirality induced in the symmetrical portion of a molecule by an asymmetric center in a different portion of the same molecule, when the latter reacts with an achiral reagent.

Obviously, both concepts are not strictly synonymous, although both are currently misused as equivalents. The term chiral synthesis, which extends and simplifies these concepts, is gaining in-

AIDS RESEARCH: More funds, coherent strategy needed

The National Institutes of Health has responded with unprecedented speed to the crisis of the acquired immune deficiency syndrome epidemic. "Never has so much been learned so quickly about any disease," William H. Danforth, chancellor of Washington University, St. Louis, told the House Government Operations Subcommittee on Human Resources & Intergovernmental Relations last week.

But, Danforth also stressed, as the AIDS research program stands on the verge of its second decade, it needs more funds—perhaps as much as 25% more than the $805 million it is getting this year. And it needs a coherent research strategy.

The hearings were called by the subcommittee chairman, Rep. Ted Weiss (D.-N.Y.), to review the results of a yearlong study of NIH's AIDS research program carried out by a panel chaired by Danforth and issued last week. The panel was organized by the Institute of Medicine, an affiliate of the National Academy of Sciences, at NIH's request.

After much debate, Danforth said, the panel decided that the current administrative structure—an "institute without walls"—that has evolved for handling AIDS research is the best mechanism possible. The panel does not recommend consolidating AIDS research under a single NIH institute, "because no one institute is broad enough to provide all of the separate strands that must come together for success in dealing with HIV [human immunodeficiency virus] and AIDS."

However, that doesn't mean the study found no need for change. Panel member Melvin M. Grumbach, Edward B. Shaw professor of pediatrics at the University of California, San Francisco, said that "without a decisive breakthrough on the immediate research horizon, there is a compelling need to strengthen and institutionalize the organizational and administrative approaches for managing AIDS research as a long-term program."

Currently, Grumbach told the subcommittee, NIH's "planning for the AIDS program is linked almost entirely to the budget process; that is, it is based on anticipated resources and not on well-defined program goals and potential scientific opportunity." The past 10 years have seen funding for AIDS research increase from 0.1% of NIH's total budget to just under 10% in 1990. However, that rapid growth seems to be over, with AIDS funding holding at just under 10% in fiscal 1991 and 1992.

The time has come, Grumbach said, for NIH "to dig in for the long haul." To the IOM panel, that means it's time for NIH to develop a five-year plan to identify AIDS-related research needs and opportunities, determine priorities and program balance, identify research fields that need to be developed, define the resources needed to carry out the plan, and monitor its progress.

To do this effectively, the study says that NIH needs to expand its AIDS Program Advisory Committee to include a broader array of AIDS-related research expertise, and needs to give that group more responsibility for broad policy advice and program surveillance. The NIH associate director for AIDS research needs additional planning and evaluation staff support and more senior scientists.

And echoing a recommendation by other review groups, the panel says the NIH director should have an annual discretionary fund of $20 million, and the authority to transfer up to 1% of each NIH appropriation account to respond rapidly to unanticipated research directions or new critical health problems. The committee also made specific recommendations on various areas of AIDS research, including vaccines, epidemiology, behavioral research, preclinical drug development, and clinical trials.

Overall, Weiss found the IOM report to be "an extremely constructive guide to improving the NIH AIDS research program," and said "it should be taken seriously by the NIH leadership and full consideration should be given to its recommendations."

Apparently, that is already happening. Anthony S. Fauci, NIH associate director for AIDS research, told Weiss that the IOM committee "made a number of constructive suggestions. Many of the recommended adjustments to the program outlined in the IOM report are already under way and others are under review for future action."

Janice Long

Funding for AIDS levels off at 10% of NIH budget

$ Millions	NIH AIDS	NIH Total	AIDS % of total
1982	$ 3.4	$3643.5	0.1%
1983	21.7	4013.1	0.5
1984	44.1	4493.6	1.0
1985	63.7	5121.6	1.2
1986	134.7	5198.0	2.6
1987	260.9	6175.0	4.2
1988	473.3	6610.4	7.2
1989	602.3	7144.8	8.4
1990	740.5	7581.5	9.8
1991[a]	804.6	8276.7	9.7
1992[b]	851.2	8774.9	9.7

a Estimate. b NIH fiscal 1992 budget request. **Source:** Institute of Medicine report "The AIDS Research Program of the National Institutes of Health"

Global plant expansions will dampen U.S. exports

Additions to global steam cracker capacity will reduce exports of plastics and intermediates and will slow U.S. production growth during this decade. The slackening growth and larger capacity will boost competition among producers worldwide, resulting in a slide in profit margins. Producers of polyethylenes, polypropylene, and polyesters and intermediates, such as *p*-xylene, will be hit the hardest, pointed out several speakers at the Chemical Management & Resources Association meeting in San Antonio, Tex., late last month. The theme of the winter meeting was growth opportunities in a changing environment.

If expansions of steam crackers are completed on schedule, total capacity will grow faster than global demand for end products using the olefins and aromatics from the crackers, resulting in pressure on selling prices and profitability. Lower profit margins could lead to shutdown of some of the old and costly-to-operate plants, offsetting the new capacity additions.

With a significant overcapacity for making the basic large-volume petrochemicals, producers will be required to adapt quickly to changing business conditions if they are to stay profitable.

The keys to survival in today's environment differ from what they were 10 years ago, says Lynn T. Bourdon III, manager of feedstocks supply at Dow Chemical. Successful ethylene producers must have three main production characteristics: First is complete coproduct integration to gain the added value of the coproducts; second is wide flexibility in using many different feedstocks, in having the facilities to deliver different feedstocks from various sources, and in accommodating the output swings that result from changes in the feedstocks; and third is having a global orientation, necessary as the U.S. imports larger quantities of hydrocarbons for all uses.

Global ethylene demand during the early 1990s forecast to grow 3.9 to 4.6% annually, says Samuel M. Weinberger, a business planner at Exxon Chemical. The recent war in the Persian Gulf could reduce growth rates to between 3.5 and 4.2%. Nevertheless, Weinberger says announced ethylene capacity expansions will average 5.5% per year between 1990 and 1995. And of the announced expansions, about half will be in the developed regions of North America, Western Europe, and Japan. Growth in demand, however, is forecast to be almost 60% in the developing regions of the world, leaving 40% of the increased demand to areas where capacity will grow 50%.

Production growth of ethylene and its derivatives will be high in China and other Asia/Pacific countries, excluding Japan. These countries won't need large imports of petrochemicals from other areas of the world. As a result, the difference between exports of ethylene derivatives and imports in the U.S. will shrink from about 2.4 billion lb of ethylene equivalents in 1990 to less than 1 billion lb in 2000, Weinberger forecasts.

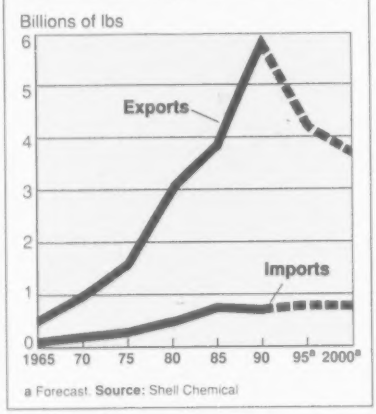
Similarly, U.S. trade in propylene derivatives will decline as global steam cracker capacity expands, according to Merritt Marbach, senior staff economic specialist at Shell Chemical. Exports of derivatives required about 6 billion lb of propylene last year; exports of propylene amounted to 500 million lb. Imports of both derivatives and propylene totaled about 1.2 billion lb in 1990. About 25% of the net trade in propylene is polypropylene, and another 15% is acrylonitrile. By the year 2000, propylene equivalents in derivatives exported will be down to about 3.7 billion lb.

This decade will produce no important supply problems for propylene, says Marbach. Chemical demand will grow at about the rate of the gross national product, and this can be met from steam cracker expansions. Thus, chemical demand for propylene produced in refineries will remain flat. However, new gasoline formulations to meet requirements of the Clean Air Act could increase demand for propylene to make alkylate.

Reformulated gasolines and demand variations for polyester fiber could affect *p*-xylene demand and supply in various ways, says James N. Raymaker, product manager for fiber intermediates at Chevron Chemical. He forecasts that, on balance, there will be a smaller merchant market for *p*-xylene, even with increased capacity. Pressures on profitability will come from tighter feedstock availability, regionalized markets causing increased freight costs, and added investment to meet higher purity specifications. With increased consumption of polyester fibers, global demand for *p*-xylene could double to 14 million metric tons by 2000.

Bruce Greek

After surge, propylene derivative exports will slump



a Forecast. **Source:** Shell Chemical

Global ethylene capacity to grow 35% through 1995

Thousands of metric tons	Capacity 1989	Capacity 1995	Steam crackers announced for 1990
U.S.	17.6	22.2	5
Canada	2.5	3.0	1
Latin America	3.0	4.4	3
Western Europe	15.7	19.7	5
Eastern Europe	7.1	7.4	6
Middle East/Africa	3.5	5.8	6
Japan	5.6	7.1	3
China	1.6	2.7	4
Other Asia/Pacific	2.7	8.0	17
WORLD TOTAL	59.3	80.3	50

Source: Exxon Chemical